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14. ABSTRACT

Summary of Findings:
Our efforts have successfully shown new technologies for increased efficiency of robust and durable thin film GaAs photovoltaic technology through enhanced light absorption and cell photocurrent as well as chemical cell edge passivation. We have shown that a combined dielectric-plasmonic grating structure can further improve the performance of solar cells by increasing absorption in thin film cells, leading to overall increases in shortcircuit

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Report Title

Routes for Efficiency Improvement in III-V Photovoltaics

ABSTRACT

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Our efforts have successfully shown new technologies for increased efficiency of robust and durable thin film GaAs photovoltaic technology through enhanced light absorption and cell photocurrent as well as chemical cell edge passivation. We have shown that a combined dielectric-plasmonic grating structure can further improve the performance of solar cells by increasing absorption in thin film cells, leading to overall increases in shortcircuit current and better angular response. Additionally, we have identified a new compound for III-V semiconductor chemical edge passivation, trioctylphosphine sulfide (TOP:S), that both eliminates size-dependent losses from exposed sidewalls and dynamically passivates regions near damages and cracks. Through this work, we enabled progress towards thinner and more durable GaAs cells that still maintain their high efficiency.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

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TOTAL:

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(c) Presentations

Number of Presentations:

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

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TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

NAME PERCENT_SUPPORTED

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Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):......

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Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

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Inventions (DD882)

Scientific Progress

Technology Transfer

Final Report

BAA Number: DARPA-BAA-09-31

Lead Organization:
California Institute of Technology

Project Title:

Routes for Efficiency Improvement in III-V Photovoltaics

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Unexpended Funds: $0
Duration of project: 12 months

PROJECT SUMMARY

Overview:

Caltech performed a 12 month effort to initiate development of three new technologies for increasing the efficiency of a robust and durable thin film GaAs photovoltaic technology, including i) plasmonic antennas for enhanced light absorption and cell photocurrent and ii) cell edge passivation in very small GaAs solar cells and iii) self-healing cell structures with chemical passivation released upon cell cracking. None of these technologies existed anywhere in the development or commercial domains for photovoltaics at the inception of the project.

1) Task 1 focused on plasmonic antenna-enhanced light absorption in thin GaAs solar cells, yielding reduced material thickness and increased open-circuit voltage. Plasmonic antennas fabricated on the front or back of the cell can enhance absorption, enabling the cell to be made thinner. Moreover, for certain applications such as deployment in unmanned aerial vehicles, there is interest in achieving constant electrical power output from a solar-powered air vehicle in level flight regardless of sun position in the sky. Thus task I focused on achieving both enhanced and angle-insensitive solar cell absorption.

2) Task 2 focused on cell edge passivation using the chemical TOP:S which reduced the surface recombination processes and leakage currents that occur on the cleaved edges of GaAs cells. While edge effects are negligible in very large cells, they can become significant in small cells. Because edge recombination and surface leakage reduce the solar cell open-circuit voltage and fill factor, development of effective cell edge passivation is important to efforts to flexible module designs that utilize very small (< 500 μm) size cells.

3) Task 3 focused on design of self-healing photovoltaic structures in which TOP:S cell chemical passivation is incorporated as part of the encapsulant material and module passivation. The chemical passivation agents were designed to be released in the cracked region when cells were been cracked and perforated. Binding of chemical passivation agents that are bound to the semiconductor surfaces exposed by cracking give rise to a reduced surface recombination velocity, thereby improving the cell fill factor and open circuit voltage

Summary of Findings:

Our efforts have successfully shown new technologies for increased efficiency of robust and durable thin film GaAs photovoltaic technology through enhanced light absorption and cell photocurrent as well as chemical cell edge passivation. We have shown that a combined dielectric-plasmonic grating structure can further improve the performance of solar cells by increasing absorption in thin film cells, leading to overall increases in short-circuit current and better angular response. Additionally, we have identified a new compound for III-V semiconductor chemical edge passivation, trioctylphosphine sulfide (TOP:S), that both eliminates size-dependent losses from exposed sidewalls and dynamically passivates regions near damages and cracks. Through this work, we enabled progress towards thinner and more durable GaAs cells that still maintain their high efficiency.

Task 1: Plasmonic and dielectric antenna-enhanced light absorption

With its band-gap at 1.42eV, GaAs is very well matched to photovoltaic conversion of the AM1.5 solar spectrum to electrical energy. Due to strong absorption of light at energies above the direct band gap, conventional GaAs cells can be a few microns thick. However techniques that enhance light absorption can enable cells that are even much thinner than 1 micron, further reducing cost and weight. In this task we investigated efficient light trapping techniques making use of scattering and light concentration properties of plasmonic and dielectric nanostructures. We demonstrated that a properly designed nanostructure can lead to improved efficiencies compared to a flat cell with an optimized antireflective (AR) coating.

Fig. 1 shows such a plasmonic structure consisting of a periodic array of Ag stripes on a silica-coated 50 nm thin Si film coated by a Silica substrate. We observed that a Ag grating structure combined with a conformal AR coating can achieve a wide-angle response over +/-45 degrees with a 30% overall increase in absorption and photocurrent over a comparable flat cell with an optimized AR coating.

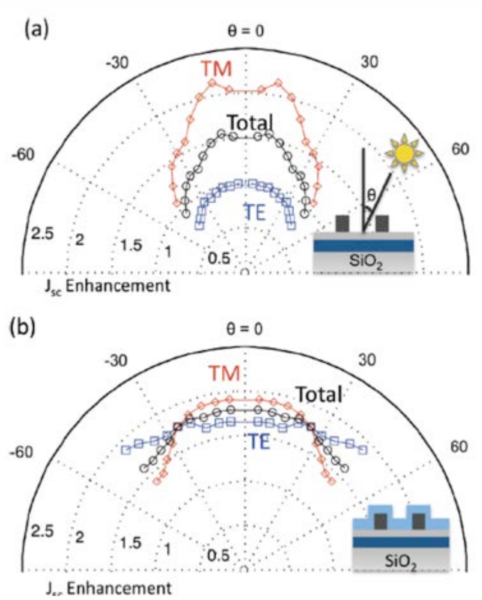

Figure 1. Angular dependence of the integrated current enhancement for (a) a grating structure and (b) a grating structure with a conformal AR coating. Both structures show enhancements for all angles considered, and the grating structure with conformal AR coating gives the largest enhancements with the least angle dependence.

Similar to plasmonic structures, a dielectric nanostructure with a properly designed morphology can act as a strongly resonant antenna and increase the light-trapping in the GaAs active material. We found that as the GaAs active layer gets thicker it is more effective to put plasmonic structures on the back of thin solar cell and instead employ dielectric particles on the front surface. To determine the optimum design parameters and understand different enhancement mechanisms for a dielectric grating/thin film structure we used a simple model system consisting of a thin GaAs cell on a silica substrate with a periodic array of a TiO_2 grating lines on top (see inset in Fig. 2). We simulated GaAs films with varying thickness (100nm-1um) and optimized grating parameters such as period, thickness and width. We found that the GaAs active layer thickness determines the dominant absorption enhancement mechanism: in ultra-thin (100-200nm) films, particle resonance coupling into waveguide modes dominates absorption, whereas for thicker GaAs films (~1um) both particle resonance and Fabry-Perot resonance effects need to be optimized in order to maximize solar absorption. We calculated the angular performance of the short-circuit current density for the optimum grating structure and compared the results to a flat GaAs cell with an optimized two-layer conventional AR coating (Fig. 2). We found that it is possible to outperform the conventional AR coating at all incident angles, with a 47% increase at 30 degrees over the bare film whereas a double-layer AR coating gives only 43% increase. Also we have shown that angular performance can be further improved by tuning the grating parameters and can have a much better performance than the 2-layer AR coating however with a slightly decreased overall performance.

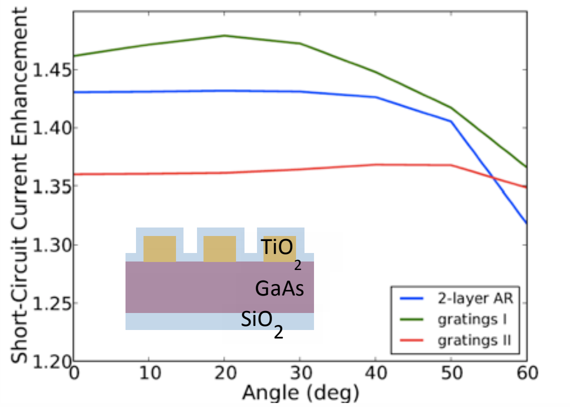

Figure 2. Comparison of integrated short circuit current density for a 1 mm thick GaAs on a SiO_2 substrate having a dielectric TiO_2 grating of on top with a flat cell having an optimized 2-layer AR coating. Dielectric grating both demonstrates a better performance for P = 400 nm period with 260 nm width by 260 nm height and also has better angular performance for P = 340 nm and 60 nm by 240 nm height and width of the grating. Gratings have conformal 100nm thick SiO_2 coating.

In order to experimentally implement our theoretical predictions, thin-film GaAs structures were fabricated using epitaxial lift-off and wafer bonding techniques. Using these techniques thin GaAs device layer with a Ni-Cu backing was transferred onto an arbitrary metal/glass substrate. The proposed surface structures are going to be fabricated using soft conformal imprint lithography (SCIL) techniques. Current studies focus on improvement of epitaxial lift-off technique, fabrication of surface structures and optical and electrical characterization of the cell performance.

Task 2: Cell Edge Passivation

In order to produce solar cells that are both highly efficient and durable, high performance cells, such as GaAs-based devices, can be made smaller ($< 1\ cm^2$) to prevent damage from cracks or impacts to the brittle semiconductor material. However, such strategies require effective electronic passivation of the exposed lateral sidewalls to prevent losses due to edge recombination. Our efforts identified new chemical agents for GaAs passivation, specifically optimized for these previously uncharacterized sidewall facets. We demonstrated that a simple treatment boosts small cell performance by reducing sidewall recombination in addition to "healing" induced fractures in thin film cells.

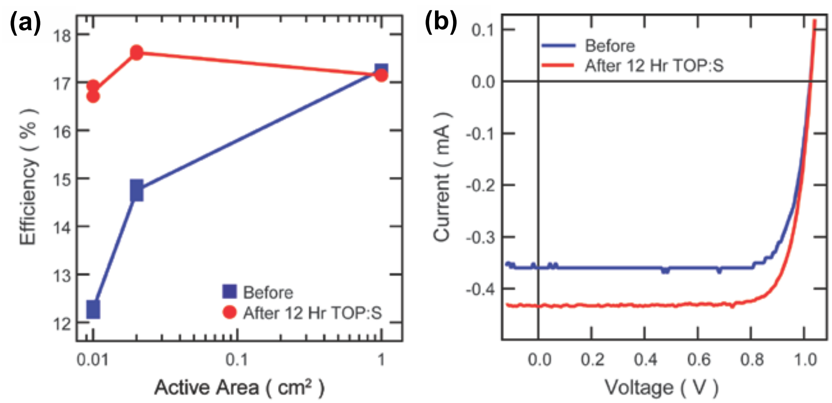

Figure 3. Size-dependent response of GaAs devices under illumination before (blue) and after (red) treatment with TOP:S. (a) Size-dependent trend in efficiency. The solid lines are a guide for the eye. (b) Representative current-voltage response of a $0.02\ cm^2$ device.

Since passivation by conventional window layers fabricated via planar epitaxial growth is difficult to achieve on sidewalls, other passivation methods, such as chemical dips, were researched. It is well known that sulfur-based compounds provide the highest quality passivation for GaAs but many effective treatments also etch GaAs and destroy materials common in solar cell production. To circumvent these challenges, trioctylphosphine sulfide (TOP:S), a ubiquitous surfactant in the nanocrystal community, was identified for the first time as a candidate for passivation of GaAs.

TOP:S was applied to a series of different sized ($1\ mm^2$, $2\ mm^2$, and $1\ cm^2$) GaAs thin film solar cells. Without passivation, a decline in efficiency was observed (Fig. 3, blue markers) with decreasing cell size. Smaller cells have a larger ratio of exposed lateral edges to active area and thus relatively more recombination sites. After submerging in TOP:S for 12 hours, the efficiency in the smallest cells greatly increased, approaching the efficiency of the largest cell. This increase is primarily due to a decrease in the sidewall recombination current, which was reduced by 80%, from 3.5 pA/cm to 0.7 pA/cm, after treatment. This performance enhancement eliminated the size-dependent losses, enabling the production of small, high efficiency cells.

Task 3: Self-Healing Photovoltaic Structures

A final study tested the ability of TOP:S to be integrated in a device structure for "self-healing" cells, or the ability to dynamically passivate facets exposed in the solar cells by the formation of cracks and damage. The collected current near an induced fracture was mapped using a confocal microscope and excitation from a 488 nm laser source. We compared this light beam induced current (LBIC) map of the fractured region before and after the device was submerged for 12 hours in TOP:S. Analysis of line scans from the LBIC measurements (Fig. 4) indicated that treatment by TOP:S reduced the surface recombination velocity (SRV) of the exposed edge from 8500 cm/s to 510 cm/s, a 94% decrease. This improvement indicates that TOP:S is an effective method for mitigating carrier recombination-related current losses at exposed sidewall facets, even from damage to the solar cell during operation.

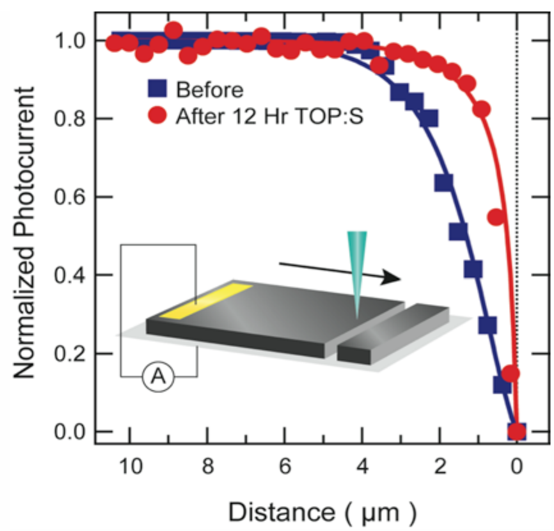

Figure 4. Light beam induced current (LBIC) profile approaching an induced fracture before (blue squares) and after treatment with TOP:S (red circles) with fits (lines).

PUBLICATIONS

1. Munday, J. N.; Atwater, H. A." Large integrated absorption enhancement in plasmonic solar cells by combining metallic gratings and antireflection coatings." *Nano Letters* 11, (6), 2195-2201 (2011).

2. Sheldon, M.T., Eisler, C.N., Atwater, H.A. "GaAs Passivation with Trioctylphosphine Sulfide for Enhanced Solar Cell Efficiency and Durability." *Advanced Energy Materials*. February (2012).

PATENTS

1. Sheldon, M.T., Eisler, C.N., Atwater, H.A. "GaAs Surface Passivation Using Sulfur- and Selenium- Functionalized Surfactants." U.S. Patent Application No. CIT 5912-P, Provisional (filing date June 20, 2011).

PRESENTATIONS

1. Pala, R., Callahan, D., Spinelli, P., Fang, A., Polman, A., Atwater, H.A. "Surface nanostructures for broadband and wide-angle response absorption enhancements in thin-film GaAs solar cells." Spring MRS. San Francisco, CA. April 2012..

2. Pala, R., Callahan, D., Spinelli, P., Fang, A., Polman, A., Atwater, H.A. "Surface nanostructures for broadband and wide-angle response absorption enhancements in thin-film GaAs solar cells." SPIE Optics and Photonics, San Diego, CA August 2012.

3. Eisler, C.N., Sheldon, M.T., Atwater, H.A. "Enhanced Performance of Small GaAs Solar Cells via Edge and Surface Passivation with Trioctylphosphine Sulfide." PVSC. Austin, Texas. March 2012.

4. Eisler, C.N., Sheldon, M.T., Kayes, B.M., Atwater, H.A. "Enhanced Performance of III-V Compound Solar Cells via Edge and Surface Passivation with Trioctylphosphine Sulfide and Related Surfactants." Spring MRS. San Francisco, CA. February 2012.

5. Sheldon, M.T., Eisler, C.N., Atwater, H.A. "Towards `Self-Healing' Solar Cells: Dynamic GaAs Passivation Using Sulfur-Functionalized Surfactants." Fall MRS. Boston, MA. November 30, 2011.